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Development of a model for the auto-ignition phenomenon in spark ignition engine operating with natural gas

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Abstract : This paper presents the development of a thermodynamic model for prediction of the auto-ignition phenomenon, applied to spark-ignition engines, and the characterization of said model, in order to accurately predict the temperature in the combustion chamber, and therefore evaluate the auto-ignition probability at a certain operating condition. From the results, can be concluded that the auto-ignition probability increases at higher intake pressures and compression ratios, and the intake temperature greatly raises the phenomenon, generating the auto-detonation at lower compression ratios. The model results are in accordance to the experimental data, and this gives the possibility to verify if a machine operating under certain conditions can be used in another place and another type of fuel without the risk of auto-ignition.

Keywords: Auto-ignition; Engine; Modelling; Polytropic process; Spark ignition.

Introduction

Recently, the auto-detonation and auto-ignition phenomena in Spark-Ignition (SI) engines have become a popular research subject, due to their potential for efficiency improvement; though these two are different processes (from a theoretical view), studies had been developed in order to correlate these phenomena [1]-[4]. Examples of this can be seen in the work of Wang [5], who established a causal relationship between auto-ignition and auto-detonation and shows their effects on the engine.

One of the main aspects of the auto-detonation analysis is the hot-spots generation. These spots are generated mainly by high-pressure waves in the combustion process. Regarding that, Terashima [6] showed by means of 1-D analysis, that the hot-spots are generated from the expansion of the ignition wave, which rebounds at the cylinder wall, increasing the chamber temperature; besides that, a numerical method was developed to establish the hot spots reactivity. In the other hand, Hajireza [7] studied the hot spots generated by the low homogeneity in the escape pressure and temperature, while Terashima and Koshi [8] showed that

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high-pressure shockwaves can also be originated in the vicinity of the ignition spark, and amplifies with their reflection at the cylinder wall, and Yao [9] analyzed the pressure distribution in the piston head by using numerical methods to model the pressure waves in the combustion chamber, which showed that the waves convergence and effects are related with the chamber geometry.

The methods for the detonation detection have been vastly studied and applying multiple procedures, Loubar [10] proposed the detonation detection by means of numerical simulation of the heat transfer from the combustion chamber to a cold water stream, measuring the temperature peaks generated from the detonations, while Ettefagh [11] establishes the measurement of the cylinder vibrations as a method to calculate the detonations in the engine.

By using alternative fuels and the exhaust gas recirculation (EGR) system, Wei [12] proposed an engine with n-butanol fuel and an EGR valve and compared with results obtained with gasoline fuel, measuring the detonation occurrence probability, which is way lower in the first case. Additional to that, Liu [13] studied the engine efficiency using a gasoline-methanol double-injection system, which lowers the detonation occurrence, and Sileghem [14] analyzed the detonation intensity in engines using a mixture alcohol-gasoline.

Besides detonation detection and alternative fuels research, there are works oriented to simulate the detonation process, as the work of Merola [15], who studied this phenomenon using 2D images to capture the combustion process in real time, compared to previous studies which were only able to establish its occurrence. To improve the quality of the simulations, Zhen [16] [17] used multi-dimensional analysis and numeric analysis on an engine with high compression ratio and fueled with ethanol, to demonstrate that the EGR, the chamber geometry design and a rich mixture lowers the pressure peaks generated by auto-detonation; in the same way, Robert [18] used LES to show the randomness of the detonations (though their locations are possibly associated with the previous ones), and Spelina [19] studied the relationship between the spark advance and the number of cycles of the engine.

The purpose of this study presented below is to carry out the characterization of the thermodynamic cycle of a spark-ignition engine, in order to accurately predict the temperature in the combustion chamber, and therefore evaluate the auto-ignition probability at a certain operating condition. The theoretical model developed, will be validated with experimental data, in order to evaluate the accuracy and reliability of the model, which is adjusted with the studied engine.

Methodology

Previous assumptions of the model

A quasi-static process what can be described as Pv^n = constant is commonly called a polytropic process. The usual processes of gas expansion or compression can't be treated as adiabatic or isothermal, but can be approximated to a polytropic process with $1 < n < k$, where k is the isentropic coefficient [20]. Taking in account this fact, it's possible to relate in a differential way the P,T and V variables in the following way:

$$\frac{dT}{T} + (n-1)\frac{dv}{v} = 0 \qquad (1)$$

$$\frac{dP}{P} + n\frac{dv}{v} = 0 \qquad (2)$$

$$\frac{dT}{T} - \left(\frac{n-1}{n}\right)\frac{dP}{P} = 0 \qquad (3)$$

By solving the former expressions, it's possible to determine the final status of the system, which allows to calculate the temperature for a fixed point of piston stroke. However, these expressions don't take in account for explicit environmental factors, as air humidity, contaminants, and the time dependence. An even deeper analysis, shows a dependence with the crankshaft rotation and heat transfer in the cylinder walls and escape gases, which are factors to keep in mind. Therefore, the model developed in this work, takes account for the heat transfer from the burned gases trapped in the TDC, which are at the escape gas temperature; this burned fraction, raises the temperature of the fresh fuel/air mixture that enters the combustion chamber during the intake process. By the definition of a polytropic process for steady-state conditions (constant heat release),

is evident that the polytropic coefficient really takes in account this phenomenon, and helps to establish that the characterization of the combustion chamber for a certain set of conditions, will allow the replication of the results for other conditions.

Due to the wide temperature ranges used in the fuel/air mixture intake (0-50°C) up the ignition point temperature (520-600°C), assuming constant thermodynamical properties (density, specific heats, etc.) would be a huge mistake; in this case, the literature [20] offers a certain number of correlations to calculate by integral form the properties for a specific fluid temperature and composition. These correlations have high exactitude, which makes them very reliable to use.

The assumptions above mentioned, should be validated in an experimental way, in order to verify if these can describe the physical phenomenon to the desired precision degree.

Development of the model

As shown previously, a polytropic process of a system is described as a pressure-volume ratio of the form

$$PV^n = Constant \qquad (4)$$

where n is a process characteristic constant. For a polytropic process between two states, the relation becomes

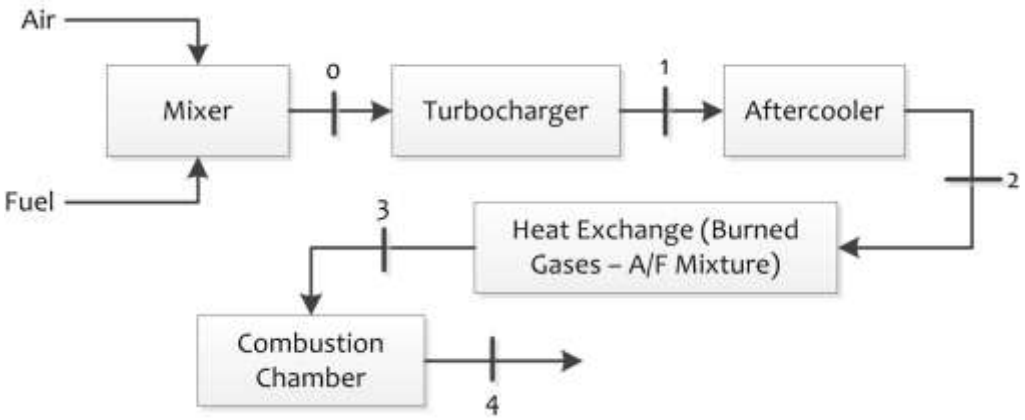
$$\frac{P_2}{P_1} = \left(\frac{V_1}{V_2}\right)^n \qquad (5)$$

If n=0, the process becomes isobaric (constant pressure), and if n=∞, the process becomes isochoric (constant volume). The former expression, is useful for any gas experiencing a polytropic process. In the same way, it's possible to relate the pressure-volume ratio with the temperature, which is the usual situation in a combustion chamber:

$$\frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{\frac{n-1}{n}} = \left(\frac{V_1}{V_2}\right)^{(n-1)} \qquad (6)$$

In order to develop expressions that describe each status in the process, a thermodynamical analysis was used, applying the previous assumptions and the polytropic process equations. Figure 1 shows a schematic diagram of the analyzed system and its intermediate points.

Figure 1. Schematic diagram of the studied steps on the engine.



At point zero (0), there's a fresh mixture air/fuel at environmental temperature and pressure (after reaching thermodynamical equilibrium during the mixing process). Then, the mixture goes to the turbocharger, which raises the discharge pressure and temperature (point 1); at this point, the characterization of the turbocharger implies the estimation of the polytropic coefficient from pressure and temperature at those points. After doing so, the compressed mixture pass through an aftercooler, which lowers its temperature at constant pressure (since the pressure drop can be neglected [21]), to reach the point 2. From that point, the mixture enters the

combustion chamber, and gets confined with residual gases from the previous cycle [22], occupying the volume between the TDC and the cylinder head. At this place (point 3), it is necessary to know the mixture and escape gases composition in order to characterize the mixture [23]. From this point, compression process starts, which is characterized by geometrical parameters of the combustion chamber and ignition point, since previous studies made clear its influence over this process [24].

Keeping the previous information in mind, it's possible to formulate the polytropic process 0-1 as

$$T_1 = T_0 \left(\frac{P_1}{P_0}\right)^{\frac{n_{01}-1}{n_{01}}} \qquad (7)$$

By assuming constant temperature drop, T_2 can be expressed as

$$T_2 = T_1 - \Delta T \qquad (8)$$

Replacing equation (8) in equation (7),

$$T_2 = T_0 \left(\frac{P_1}{P_0}\right)^{\frac{n_{01}-1}{n_{01}}} - \Delta T \qquad (9)$$

where n_{01} is the polytropic coefficient for the turbo-compression process, and ΔT is the temperature drop at the aftercooler.

For the process between points 2-3, it's necessary to take account for the heat transfer from the residual gases, and the temperature rise originated by this; thermodynamically, it can be expressed as

$$\dot{Q}_{2\text{-}3} = -\dot{Q}_{gases} \qquad (10)$$

In the same way, an equivalent expression of equation (10) is

$$m_R Cp_R (T_e - T_3) = m_m Cp_m (T_3 - T_2) \qquad (11)$$

where T_e is the escape gases temperature, states (R) are for the escape gases, and states (m) are for the fresh mixture that enters the combustion chamber. From equation (11), equilibrium temperature T_3 is calculated as

$$T_3 = \frac{\frac{m_R Cp_R}{m_m Cp_m} T_e + T_2}{1 + \frac{m_R Cp_R}{m_m Cp_m}} \qquad (12)$$

The mass of the mixture and escape gases, can be related to its volume by the expressions

$$m_R = \rho_R V_c \qquad (13)$$

$$m_m = \rho_m V_d \qquad (14)$$

where the density is directly related to mixture composition and it's calculated according to the total mixture fraction. Replacing the equations (13) and (14) in (12), the following expression can be obtained:

$$T_3 = \frac{\frac{\rho_R V_c Cp_R}{\rho_m V_d Cp_m} T_e + T_2}{1 + \frac{\rho_R V_c Cp_R}{\rho_m V_d Cp_m}} \qquad (15)$$

The compression ratio is, by definition [20],

$$r_c = \frac{V_d + V_c}{V_c} \qquad (16)$$

where V_c is the combustion chamber volume and V_d is the volume displaced by the piston. Then it is possible to obtain the following expression from equation (16)

$$\frac{V_c}{V_d} = \frac{1}{r_c\text{-}1} \quad (17)$$

By substituting equation (17) into equation (15), the equilibrium temperature T_3 can be expressed as a function of the compression ratio:

$$T_3 = \frac{\frac{\rho_R Cp_R}{\rho_m Cp_m}\left(\frac{1}{r_c\text{-}1}\right)T_e + T_2}{1 + \frac{\rho_R Cp_R}{\rho_m Cp_m}\left(\frac{1}{r_c\text{-}1}\right)} \quad (18)$$

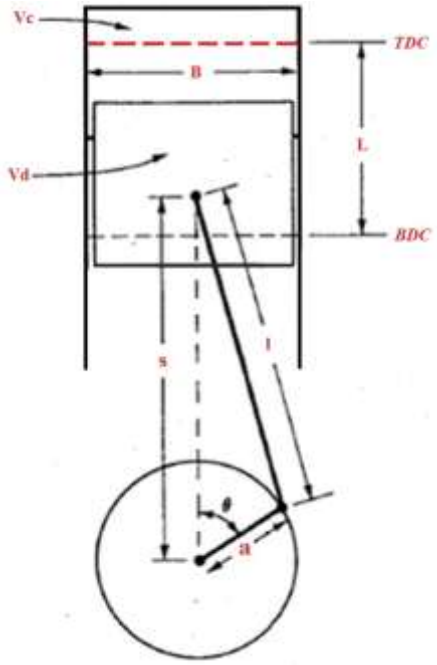
For the polytropic compression process (3-4), it's well known the following expression:

$$T_4 = \frac{T_3}{\left(\frac{V_4}{V_3}\right)^{n_{34}\text{-}1}} \quad (19)$$

To calculate the volume V_4 taking in account its dependence with time, it is necessary to do a geometrical analysis of the engine. By using a scheme similar to Figure 2, the piston position *s* can be calculated by the expression

$$s = a\cos\theta + (l^2 - a^2 sen\theta)^{\frac{1}{2}} \quad (20)$$

Figure 2. Geometry configuration for the cylinder, piston and connecting rod (B=piston bore, L=stroke, l=rod length, a=crankshaft pin radius, θ=crankshaft angle)



And the displaced volume can be described as function of the position *s*, as follows:

$$V_4(\theta) = V_c + \frac{\pi B^2}{4}(l + a - s(\theta)) \quad (21)$$

Substituting the equation (20) in (21), the following equation is obtained:

$$V_4(\theta) = V_c + \frac{\pi B^2}{4}\left(l + a - a\cos\theta - \left(l^2 - a^2 sen^2\theta\right)^{\frac{1}{2}}\right) \quad (22)$$

Using the ratio of the connecting rod length to the crankshaft radius, and the definition of the displaced volume,

$$R=\frac{l}{a} \qquad (23)$$

$$V_d=\frac{\pi B^2 L}{4}=\frac{\pi B^2(2a)}{4} \qquad (24)$$

On the equation (22), yields the expression

$$V_4(\theta)=V_c\left(1+\frac{V_d}{2V_c}(R+1-\cos\theta-(R^2-\text{sen}^2\theta)^{\frac{1}{2}})\right) \qquad (25)$$

Which if substituted in the equation (21) allows to obtain a unique equation for T_4:

$$T_{ignition}=T_4=\frac{\frac{\frac{\rho_R Cp_R}{\rho_m Cp_m}\frac{1}{(r_{c-1})}T_e+\left(T_0\left(\frac{P_1}{P_0}\right)^{\frac{n_{01}-1}{n_{01}}}-\Delta T\right)}{1+\frac{\rho_R Cp_R}{\rho_m Cp_m}\frac{1}{(r_{c-1})}}}{\left(\frac{1}{r_c}\left(1+\frac{r_c-1}{2}(R+1-\cos\theta-(R^2-\text{sen}^2\theta)^{\frac{1}{2}})\right)\right)^{n_{34}-1}} \qquad (26)$$

where the polytropic coefficients n_{01} and n_{34} should be adjusted for the studied engine.

Results and experimental validation

With the equations (8), (10), (19) and (22), it is possible to calculate the temperature at any place of the process shown in Figure 1. However, since the auto-detonation phenomenon is directly related to the temperature in the combustion chamber (T_4), Figures 3-5 show this temperature as function of different compression ratio and intake pressure, for a specific intake temperature. For comparison purposes, the auto-ignition temperature was added to the plot, and to show the intake temperature influence over the combustion chamber, surface response plots for a constant compression ratio are shown in Figure 6.

Figure 3. Combustion chamber temperature vs. intake pressure (Intake temperature 20°C)

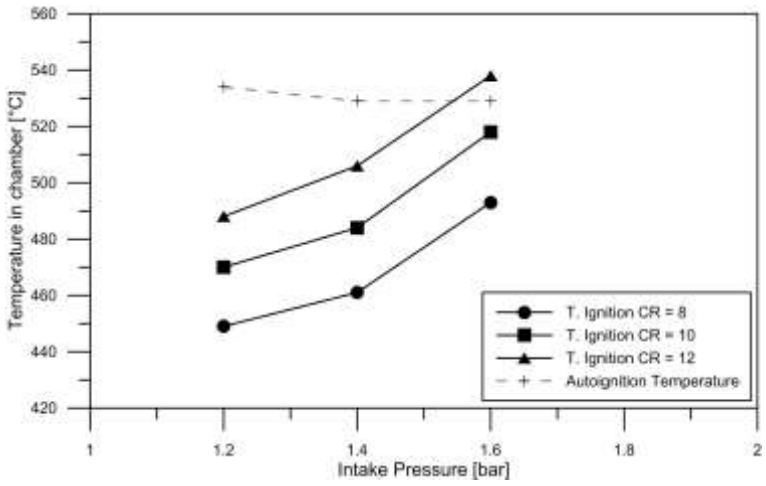


Figure 4. Combustion chamber temperature vs. intake pressure (Intake temperature 30°C)

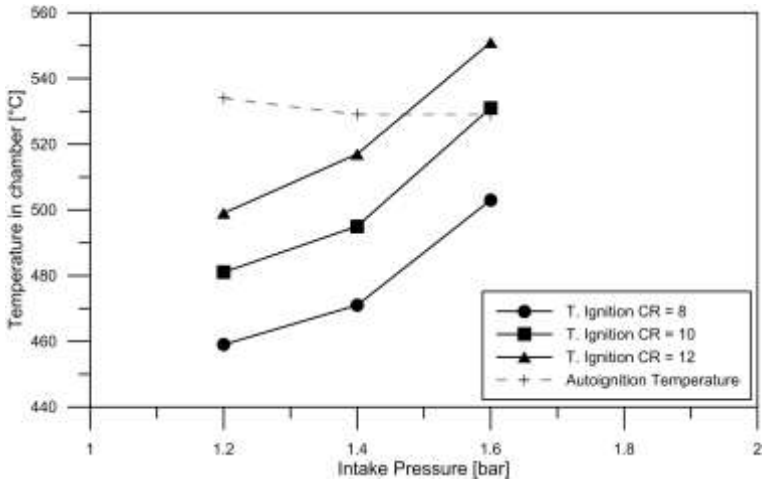


Figure 5. Combustion chamber temperature vs. intake pressure (Intake temperature 40°C)

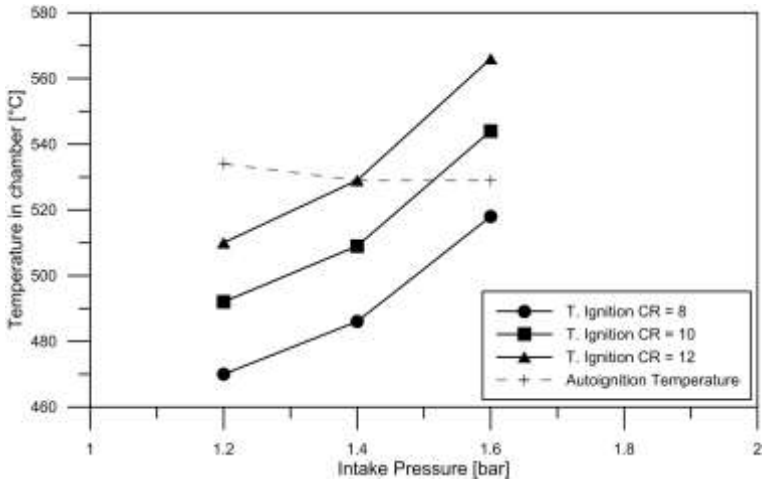
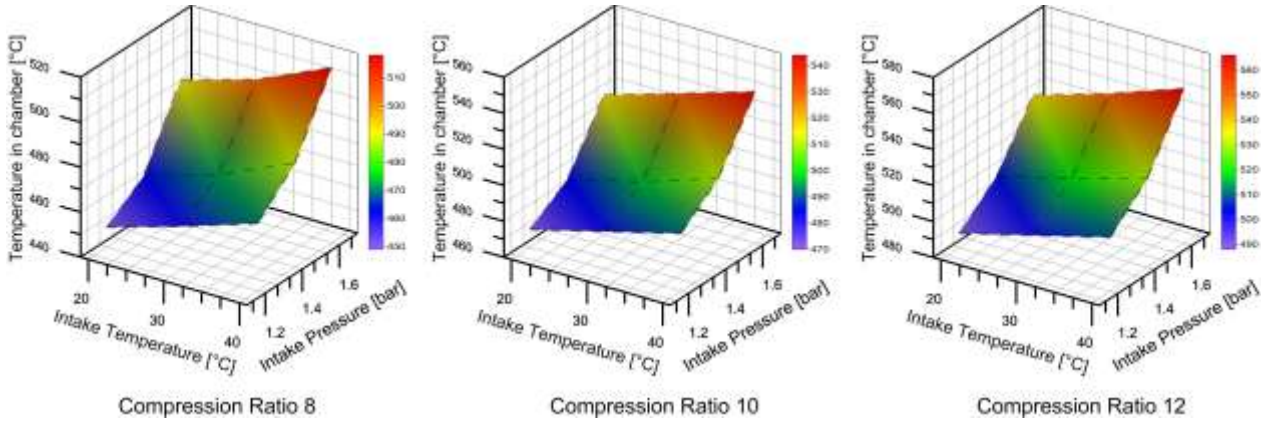
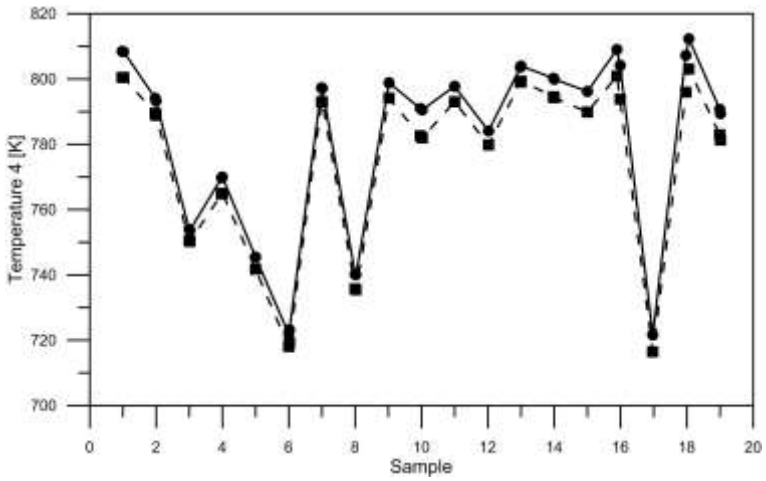


Figure 6. Response surface plots for constant compression ratio



From these graphs, it can be concluded that the auto-detonation probability increases at higher intake pressures and compression ratios, and the intake temperature greatly raises the phenomenon, generating the auto-detonation at lower compression ratios (as shown in Figure 5). For the validation, a QSV91 spark-ignition engine was used, with adjusted coefficients n_{01}=1.381 and n_{34}=1.364. The comparison between the experimental data and the adjusted model, is shown in Figure 7. It is observed that the model didn't generate outliers, as it has the same behavior of the real process, which is to be expected of a thermal machine characterization in order to extrapolate its behavior in different working conditions. Besides, the usefulness of this process resides in the fact that concepts of similarity can be applied to thermal machines [25] and many of them handle the same parameters among themselves despite being built by different manufacturers, which allows to generalize the procedure.

Figure 7. Experimental data vs. mathematic model



Sample 10 was carried out with a relative humidity of 60%, which may explain the deviation between the estimated value and the real value. Despite this deviation, the relative error for this measurement is 1.1 %, which is very low considering that the model does not consider the influence of humidity in the intake air entering the engine.

Conclusion

The study carried out important conclusions about the auto-detonation phenomenon. The influence of intake temperature and pressure on the auto-ignition temperature was verified, and it was corroborated that, keeping the other parameters constant, a 10% decrease in the intake pressure leads to an increase of 4% in the intake temperature, and this above implies that if an engine operating in Barranquilla (Colombia) reaches a temperature at the ignition point 10 °C below the fuel auto-ignition temperature and it is transferred to Bogotá with identical operating conditions (except for the environmental pressure), auto-detonation occurs. In addition to this, as a lower intake pressure is handled (about 25% less), in Bogota (Colombia) the effective average pressure will decrease by around 15%, which would lead to the engine loss of approximately 20% of its maximum power [26].

From Figure 7, it was observed that the deviation average error between each one of the stages of the cycle in analysis did not exceed 1%, which sheds light on the effectiveness of the designed method. This work, was based on a characterization – prediction method, where an engine is studied under certain conditions and the model given is used to describe the behavior of the temperature at the ignition point for different conditions. This gives the possibility to verify if a machine operating under certain conditions can be used in another place and another type of fuel without the risk of auto-ignition, by finding if the temperature at the ignition point reached the auto-ignition temperature of the air/fuel mixture, which is defined by the composition of the gas.

The calculation of the experimental polytropic coefficients leads to very useful results in practice. If the study were extended to a general characterization of engines (proposed in future work) it is possible to obtain a database of the most commercial engines operated with natural gas, in order to verify the interchangeability taking into account the results obtained, where the coefficient does not vary significantly while the engine power and the engine speed remain constant.

Another verified fact was that there is no significant variation in the composition of the exhaust gases over time, as long as the engine speed (RPM and Power) is not changed, which allows the analysis to be simplified, since the composition is fixed of the exhaust gases according to the manufacturer's technical sheet (to comply with emission regulations). Besides, the results obtained verify an assumption made at the beginning of the formulation of the model (the relative humidity was not significant over the model formulation), due to the high fuel volumes handled, the particulate filtering system used in this type of engines, and the compression process in the turbocharger, which generates a temperature increase that helps to mitigate this factor.

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